Driving Sustainability

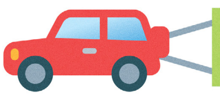
In the future, city transportation systems will be very different. From sustainably sourced materials to automated vehicles, Los Alamos scientists are helping drive transportation technology toward an ecofriendly future.

When something is old and used up we throw it away. We throw away pens, shoes, and umbrellas; we throw away suitcases, beds, and cars. Wait, cars? Yes, cars. Although we don't actually put a car on the curb for the garbage truck, there's little choice for cars that are old and used up but to be junked.

Some materials, such as metals, get recycled, while others, such as tail lights, can be reused. But after the recyclables have been recycled and the reusables have been reused, what remains gets shredded and interred in landfills. With a typical lifetime of about 200,000 miles, Americans throw away roughly 12 million cars every year. Waste reduction and sustainability are moving fast in other sectors but have some catching up to do when it comes to the automotive industry. From concept to scrapyard, there's plenty of room for improvement in how cars are built that can help extend their lives and reduce their waste. Scientists across Los Alamos National Laboratory are participating in several collaborations and national consortia to work all the angles and build inroads toward a more sustainable future of driving.

The zero-waste movement is gaining traction and infiltrating the mainstream. Cities are running out of places to put trash and running low on materials to make new stuff to replace trash, so many are going green to reduce their refuse. Cities, families, and individuals are joining ranks in reducing landfill contributions incrementally over about 20 years. The end goal is 100 percent waste diversion, where nothing goes to the landfill. Plastic grocery bags and take-out boxes are verboten, recycling is compulsory and broadly inclusive (not just soda cans and newspapers anymore), and some cities even have daily curbside pickup of food scraps for community composting programs. Companies, too, are getting on board, redesigning their products and packaging to minimize waste. The old mantra "reduce, reuse, recycle" now includes "repurpose, reclaim" and in some instances "replace," with respect to using alternate sources and materials that are more sustainable and future-friendly. So, what does that mean for cars?

Sustainability in transportation is a many-faceted challenge. The fossil fuels that power conventional cars are limited in supply, as are some of the materials used in hybrid engines. Cars are made from steel, which is heavy, and heavy things require more fuel to accelerate. However, lighter things are more easily damaged and are therefore frequently repaired or replaced. Many parts are made of plastic, which also draws on the finite supply of oil for its production. And of course, greenhouse gases produced from combusting fossil fuels contribute to climate change and air pollution, while discarded plastic and spilled oil pollute the land and water. Sustainable transportation as a paradigm has the charge of maintaining our present standards of travel—speed, safety, comfort, affordability—while no longer relying on finite resources like oil or causing harm to the environment. That's a tall order but also a necessary one.



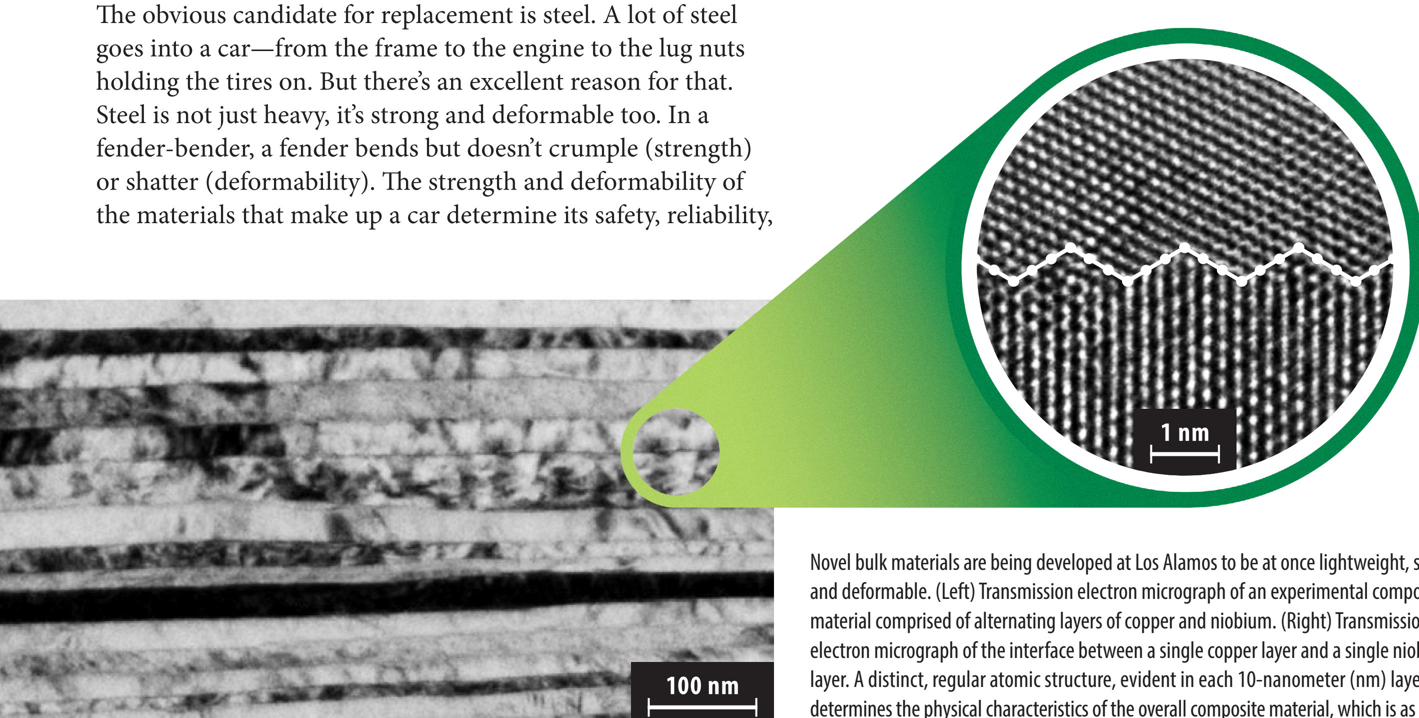
When a car dies, much of its matter gets interred in a landfill.

Lightening the load

One way to reduce a car's environmental footprint is to change what it's made of. For every hundred pounds of weight shed, a car gets a fuel-economy boost of 2 percent. But if a car is too light it will feel like a shoebox on wheels, and it may perform about as well. So it's a matter of finding the sweet spot between the performance and safety of heavier cars and the fuel economy of lighter cars. With this in mind, much effort is going into finding safe ways of lightweighting tomorrow's cars. The obvious candidate for replacement is steel. A lot of steel goes into a car—from the frame to the engine to the lug nuts holding the tires on. But there's an excellent reason for that. Steel is not just heavy, it's strong and deformable too. In a fender-bender, a fender bends but doesn't crumple (strength) or shatter (deformability). The strength and deformability of the materials that make up a car determine its safety, reliability, and performance. So materials with strength and deformability like steel that weigh less than steel would be ideal. But lightweight, high-performance materials like titanium and carbon fiber are expensive. Race car drivers or custom car builders may be willing to pay for these luxury materials to improve the performance of their vehicles, but average American car buyers are not.

Aluminum is being used by major car companies to replace steel wherever possible. Some perks of using aluminum are that it's much lighter than steel, it has high deformability, and the technology and infrastructure for aluminum recycling is well established. But aluminum has some problems too. It's not very strong, and it can be difficult to join pieces together. Welding aluminum is tricky for a number of reasons, including its low melting point, its propensity to harbor impurities, and the fact that aluminum alloys can only be welded to like alloys. Aluminum is also energy intensive to machine or cast, and high heat can weaken it, sometimes forcing manufacturers to resort to using rivets or adhesives to join pieces together.

Magnesium is another metal that is receiving a lot of attention for lightweighting cars. Magnesium has properties that are similar to those of aluminum, but it is 33 percent lighter, easier and less energy intensive to machine or cast, and can be more corrosion-resistant than aluminum. And like aluminum, magnesium has some problems; chief among them are its limited strength and formability and its high flammability. So while magnesium might work for, say, the rims of a tire, it might not be a good choice for the chassis.



Novel bulk materials are being developed at Los Alamos to be at once lightweight, strong, and deformable. (Left) Transmission electron micrograph of an experimental composite material comprised of alternating layers of copper and niobium. (Right) Transmission electron micrograph of the interface between a single copper layer and a single niobium layer. A distinct, regular atomic structure, evident in each 10-nanometer (nm) layer, determines the physical characteristics of the overall composite material, which is as strong as tool steel, despite being comprised of two relatively soft metals.

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But maybe the best lightweighting solution can't be found in any extant metal. Maybe it lies in brand new materials. Researchers at Los Alamos's Center for Integrated Nano-Technologies (CINT) are working on creating materials that embody all of the desired features, being at once lightweight, strong, deformable, and environmentally friendly. For example, they've developed a composite material comprised of alternating layers of copper and niobium. Both are soft metals, so they're easy to work with, and they don't mix chemically, so the layers, despite being only 20 atoms thick, remain discrete. This is key because the material as a whole will draw its properties from atomic interactions at the interfaces of the layers, so the layers need to be controlled at a very fine level. The result is a composite that possesses strength comparable to that of the steel used for high-quality hand tools, even though it is constructed of two soft materials. This particular material is too expensive to be a steel replacement itself, but CINT scientists are using it to understand the physical interactions that give materials their strength.

"We're making materials that are ten times stronger than what is commonly available," explains Los Alamos scientist Nathan Mara. "But the big issue is that the manufacture of these materials is centered around the microelectronics industry, which requires thin films. For the automotive industry we need to make much larger sheets, rods, and tubes, which requires a novel manufacturing method." Through a process similar to the ancient technique used to produce Damascus steel for swords (repeated folding and flattening), Mara and others at CINT can produce pieces of the copper-niobium composite metal about the size of a ski. While it's not exactly a sedan side panel, it's the bulk production that's important, and they've just about got that down.

Another material being developed at CINT is comprised of nanometers-thin layers of aluminum and titanium nitride, a strong but brittle ceramic. The metal-ceramic composite material is lightweight and has the best properties of each of its components: the high deformability of aluminum and the strength of titanium. However, it could just as easily have been the worst of both worlds: a weak and brittle material. The way they decide which materials to actually synthesize is through extensive modeling. By looking at the physical characteristics of component materials, like deformability, crystal structure, and stiffness, a computer model can predict what sort of behavior a composite material might exhibit. So far, the models have been right and have led the scientists to some promising new materials.

Extensive integrative modeling also goes into understanding how to maximize a material's performance through the manipulation of its geometry and microstructure. Vehicle lightweighting isn't only about the composition of materials; it also has to do with their configuration. For example, using thicker cross sections of lightweight materials can increase their strength, while thinner cross sections of very strong materials can reduce their weight. Scientists at Los Alamos are developing and characterizing advanced high-strength steels that can do the same duty as conventional materials but with thinner cross sections and different geometries, aiding in keeping weight down while maximizing performance.

For every hundred pounds of weight lost, a car's fuel economy gains 2 percent.

Los Alamos National Laboratory is one of ten national labs participating in a new federal initiative to lightweight America's cars: the Lightweight Materials National Laboratory Consortium, or LightMAT, is part of the U.S. Department of Energy's (DOE) Clean Energy Manufacturing Initiative and is funded by the Office of Energy Efficiency & Renewable Energy (EERE). The goal of the Clean Energy Manufacturing Initiative is to boost the productivity and competitiveness of U.S. clean energy technologies in the world market. To that end, the mission of LightMAT is to enable the automotive industry to use some of the unique scientific and technical resources related to lightweight materials that exist within the national labs.

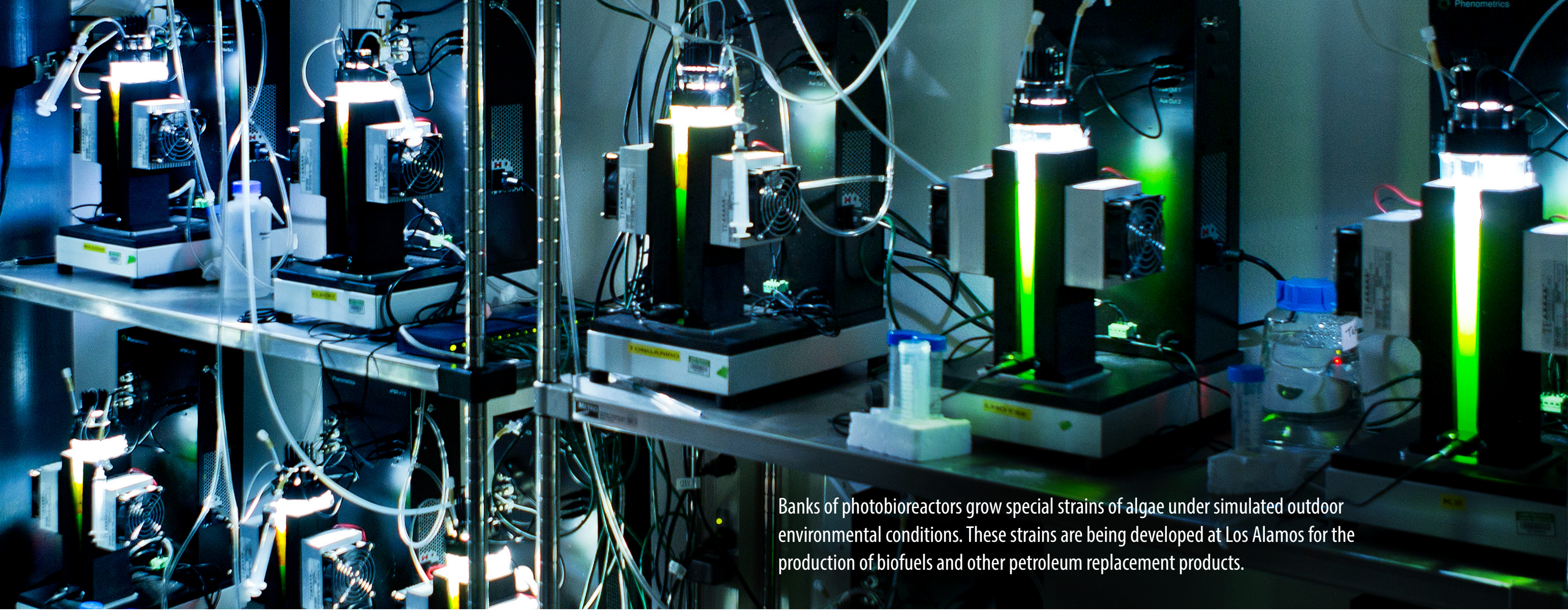
Los Alamos's Ellen Cerreta is on the LightMAT steering committee. She explains how it will work: "LightMAT offers a catalogue of capabilities that come from research and development at our national laboratories. These capabilities can be applied to challenges associated with lightweighting and will facilitate the inclusion of lightweight materials in automobiles. Through this catalogue, the automotive industry can directly access these capabilities to address their specific research needs." The immediate focus will be cars and trucks, but because the technologies are broadly transferable, buses, trains, boats, and planes will also be losing some weight in the near future.

Just one word

Plastics.

What about plastics? Each year, cars contain less metal and more plastic, so it would seem plastics need to get green too. Technically speaking, plastics are a group of malleable, moldable materials that contain synthetic or semisynthetic organic compounds usually derived from petrochemicals. Generally speaking, plastics come from oil.

Plastics are great because they are lightweight, strong, deformable, waterproof, versatile, cheap to make, and easy to work with. With all of those advantages, plastics can't be made pariahs simply because they come from oil, but not coming from oil would be even better. Los Alamos bioenergy scientists are working on petroleum replacement products (PRPs),



Banks of photobioreactors grow special strains of algae under simulated outdoor environmental conditions. These strains are being developed at Los Alamos for the production of biofuels and other petroleum replacement products.

that is, alternate sources for products traditionally made from petroleum, such as nylon, which is used in auto upholstery (among a great many other things).

"The nylon that could be made would not be a new nylon," emphasizes Los Alamos bioscientist Taraka Dale, "it would be made with the same chemicals that come out of a barrel of oil. This nylon would work the same and feel the same in your hand, because it would be the same material. It's the source that would be different."

Nylon comes from adipic acid, which usually comes from oil. But Los Alamos is collaborating with the National Renewable Energy Laboratory (NREL) on ways to get adipic acid and its biological precursor, muconate, from biomass—that is, plant parts available in large quantities that aren't otherwise needed for food. The approach entails breaking down the bonds of the biomass into sugars, which small organisms like bacteria or yeast can take up and metabolize, releasing muconate or adipic acid as a metabolic product. By modifying, inserting, or deleting genes in the bacteria or yeast, the researchers aim to make industrially relevant quantities of these precursors. Once they have adipic acid, the process of making nylon is the same as with adipic acid from crude oil.

Plastics are too good to be made pariahs simply because they come from oil.

Adipic acid is just one example, however. The Los Alamos and NREL team has joined with seven other national labs in a new, collaborative synthetic biology effort called the Agile BioFoundry, funded by the Bioenergy Technologies Office under the EERE. The Agile BioFoundry ultimately plans to make replacement versions of many other kinds of plastic materials that go into a car—things like floor mats, dashboards, sun visors, consoles, door handles, bumpers, hoses, and reservoirs, just to name a few. Even more importantly, the Agile BioFoundry aims to establish a new, generalizable platform that can rapidly design, build, and test new microbial strains and metabolic pathways for making a broad range of PRPs. This platform will help reduce both the cost and time-to-market for these PRPs, enabling the BioFoundry to meet its goal of rapid scale-up while maintaining the economic viability and sustainability that are central to its vision. Though other communities will almost certainly be interested in the Agile BioFoundry's concept for PRPs, its initial focus will be transportation.

Building a lighter, greener car is paramount to sustainable transportation. But that's just half of the equation; the other half is fixing the fuel problem. Fuel cells are the transportation fuel of the future, but in the meantime, fossil-free fuels are being developed to work in the cars of today. Algae is a promising form of biomass that can be used for fuel and PRP-coproduct production, and Los Alamos has built up considerable expertise in manipulating algae strains in an effort to make fuel precursor molecules in large enough quantities to be economically viable. Algae produce more oil per land area than other oil-producing plants (palm, soy, safflower, etc.) and can grow on marginal lands in marginal water, making them ideal candidates for a renewable source of energy-dense liquid fuel. Recent algae achievements at Los Alamos include increasing growth rate, increasing oil content, broadening the potential for coproduct production, developing energy-conserving harvesting techniques, and sequencing the genomes of several new potential algae production strains. [*To learn more about algal biofuels at Los Alamos, see "Seeing Green: Squeezing Power from Pond Scum" in the January 2012 issue of* 1663.]

Fuel cell ins and outs

Fuel cells have been around for more than 150 years. They come in several varieties and have been developed for diverse purposes. The space shuttles got electricity in part from fuel cells, as did the Gemini and Apollo spacecraft of the 1960s and 1970s. In the late 1970s, Los Alamos began its program for polymer electrolyte membrane fuel cells, or PEM fuel cells, and the program is now one of the Laboratory's longest-running programs. (Alternatively, PEM stands for proton exchange membrane, but both names refer to the same device.) PEM fuel cells are the most promising for cars, and most major car companies have their own PEM fuel-cell programs. There is little doubt that this technology will power our cars in the future.

A fuel cell is similar to a battery—both devices employ two electrodes (anode and cathode) to use the energy in chemical bonds to drive electrons through an external circuit, creating the electricity that powers a device. A battery contains a limited quantity of chemical reactants to supply electrons, and when the charge stored in those reactants is used up, the battery is discharged. On the other hand, fuel-cell electrodes do not store any charge and can produce power as long as reactants are supplied to the fuel cell, which is limited only by the size of the fuel tank. Fuel cells typically use hydrogen as fuel, which can be made from renewable resources, resulting in electricity being produced with water as the only emission. Moreover, the refueling time and range of a fuel-cell vehicle is comparable to that of a gasoline vehicle.

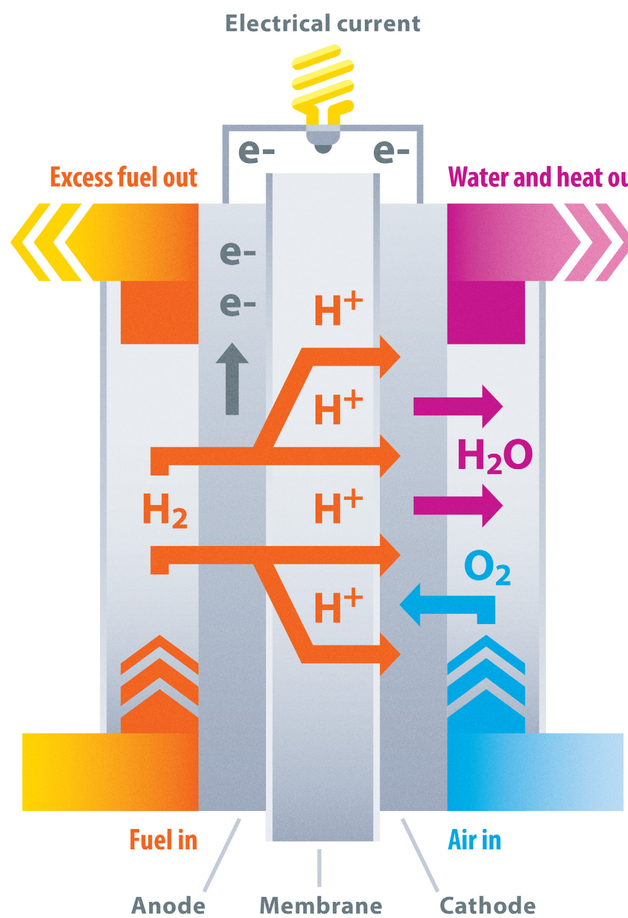
In a PEM fuel cell, hydrogen atoms enter the anode side of the cell and are dissociated with the help of a catalyst into negatively charged electrons and positively charged hydrogen ions (protons). The protons pass easily through a special electrolyte membrane that separates the anode from the cathode. Meanwhile the electrons, which are generated at the anode but can't pass through the membrane, travel along an external circuit, through whatever electrical system the fuel cell is powering, to the cathode side where they rejoin the protons and react with oxygen to produce water. The chemistry is compelling indeed—hydrogen plus oxygen make water, what could be greener than that? But there are still challenges to overcome.

The main fuel-cell challenges at present are cost and durability. One speed bump on the road to sustainability is the cost of certain fuel-cell components. A catalyst is needed on both sides of the fuel cell to facilitate one reaction at the anode and another reaction at the cathode. And as bad luck would have it, the best catalyst by far is one of the most expensive metals in the world: platinum. About 40 percent of the cost of a fuel cell comes from the platinum. Contemporary cars use platinum too—roughly 3–7 grams go into a typical catalytic converter. And while a single fuel cell uses much less than that, once fuel cells start stacking up, as they must to power a car, the quantity of platinum becomes an issue.

The ElectroCat Consortium is a product of the DOE's Energy Materials Network Initiative, in which Los Alamos has partnered with Argonne National Laboratory to get fuel cells past the platinum problem. The quantity of platinum in a fuel cell has to come down in order for fuel-cell technology to be cost-competitive with the internal combustion engine. Platinum is used in both the anode and cathode, but because the cathode contains considerably more, the focus for now is on reducing or replacing platinum there without losing performance or durability. The job that platinum does at the cathode is to split the oxygen molecule to facilitate its combination with the hydrogen ion and electrons to produce water.

Among other ElectroCat efforts, Los Alamos researchers are working on optimizing the production and performance of non-platinum-group metal catalysts. The researchers have developed a methodology that uses nitrogen–transition-metal–carbon catalysts for the electrochemistry on the cathode side. Depending somewhat on which transition metal is used in the catalyst being tested, the researchers can achieve high power output, good efficiency, and promising durability.

One potential way to move away from a platinum catalyst is to operate fuel cells under basic, or alkaline, conditions. Fortuitously, non-platinum-group metal catalysts perform as well, and even better in some cases, than platinum does in an alkaline environment. However the lack of a suitable membrane that has high conductivity and stability under alkaline conditions has hindered the development of these fuel cells. But in a recent DOE Advanced Research Projects Agency-Energy project, a Los Alamos experimental membrane outperformed all its competitors in very alkaline conditions.



Schematic of a polymer electrolyte membrane (PEM) fuel cell. A PEM fuel cell has two sides, each with an electrode (anode and cathode), separated by a polymer electrolyte membrane that keeps the chemistry on the two sides from mixing. The fuel (hydrogen gas) is channeled into the anode side and air (containing oxygen) is channeled into the cathode side.

Another problem plaguing progress is the tendency of the membrane and catalyst materials to degrade under operating conditions. The Fuel Cell Consortium for Performance and Durability (FC-PAD) includes several national labs as well as partners in industry and academia working together to commercialize low-platinum fuel cells. This Los Alamos-led consortium was assembled to address the durability challenge head on.

FC-PAD is evaluating state-of-the-art commercial electrocatalysts under relevant conditions to quantify how well they perform. It's not enough to know under what conditions a material degrades; developers also need to know why and how the degradation occurs. Then commercial catalyst makers can take that data and improve their products accordingly, or operating procedures can be developed to minimize the degradation. In addition to characterizing materials already on the market, FC-PAD scientists are testing pre-commercial products that they are trying to get to market and also conducting fundamental research toward design principles for new materials.

"We know how to make durable fuel cells," says Los Alamos fuel-cell program manager Rod Borup, "but we don't know how to make them at a cost that would enable mass commercialization." FC-PAD is trying to reduce the quantity of expensive materials like platinum by optimizing the fuel cells' structure to increase the performance of the catalyst.

Even beyond the scope of FC-PAD, laboratory scientists are working on a whole new class of PEM fuel cells to improve fuel-cell functionality. The two main types of PEM fuel cells on the market today are low-temperature PEM fuel cells, which work best below 80°C, and high-temperature PEM fuel cells, which work best above 160°C. That leaves a big gap in fuel-cell functionality.

"This is a bad place to have a functionality gap, because this temperature regime can relax certain engineering constraints for fuel cells," explains Andrew Dattelbaum, the Los Alamos Materials Synthesis and Integrated Devices group leader. "So to reduce the overall system costs, we would really like to develop devices that function well in that temperature range." Prototype fuel cells using an experimental new membrane material developed at Los Alamos recently demonstrated excellent performance and durability across a larger temperature range, from 80°C to 200°C, handily filling in this functionality gap.

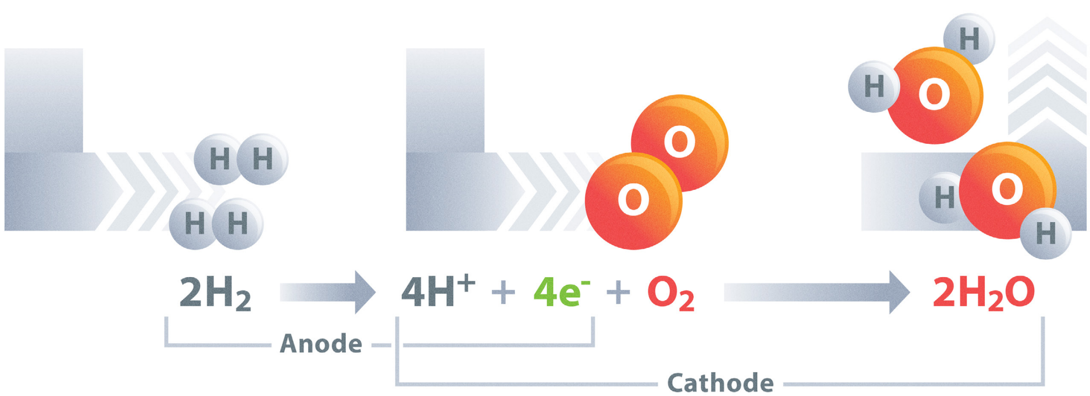
Fuel cells will undoubtedly power our cars in the future.

The final roadblock to consider for fuel-cell vehicles is the fuel-cell fuel itself: hydrogen. Presently, pure hydrogen gas, or H_2, is acquired by steam reforming of methane—reacting methane with steam at high temperature. Methane is a fossil fuel, so as long as the hydrogen in PEM fuel cells comes from methane, the fuel cells aren't completely sustainable. However, the greenhouse-gas emissions associated with steam reforming of methane are half of what conventional gasoline-powered cars produce, so even though it's just a stepping stone to true sustainability, it's a cleaner way of getting there.

Methods do exist for obtaining pure hydrogen gas that do not involve fossil fuels—electrolysis, for example, which uses electricity to split water into hydrogen and oxygen. But these methods are still cost-prohibitive; Los Alamos and other national labs are working to reduce the cost of renewably sourced hydrogen, which would help reduce the greenhouse-gas emissions of the entire energy sector.

Steam reforming, in addition to being fossil-fuel dependent, also presents a practical challenge to fuel-cell designers. The process isn't 100 percent efficient—a small proportion of other gaseous molecules remain in the hydrogen as impurities. These impurities, such as carbon monoxide and hydrogen sulfide, interfere with the precious platinum, covering its surface and thus poisoning it. This reduces the efficiency of the fuel cell and its lifespan too. As Los Alamos scientists work to develop new electrocatalysts, they are also working to understand how these materials will be affected by impurities in the hydrogen fuel. For example, for each type of impurity, how much can a fuel cell tolerate? Understanding that will help guide new hydrogen purification methods as well as the development of new catalyst materials.

Ultimately, all this fuel-cell technology has to be brought to market if it's to do any good. In order to help companies make maximum use of the fuel-cell research being done at Los Alamos, the DOE has set up a small business voucher program.



The chemistry inside a fuel cell is simple and compelling: Hydrogen is dissociated into electrons and hydrogen ions in the anode. The electrons provide electrical power and are then recombined with the hydrogen ions in the cathode, where oxygen is added, creating water as the only emission.

Automated vehicles, or self-driving cars, have tremendous potential for streamlining cities' transportation systems and boosting their occupants' quality of life. A city in which human-driven cars were replaced by automated vehicles may experience some impressive improvements: traffic jams and collisions could be largely avoided, fuel and time could be largely conserved, and people who can't drive now—blind people, young people, infirm people, intoxicated people—would be able to get where they need to go without endangering themselves and others. In order to quantify these hypothetical improvements, Los Alamos is bringing its error quantification and systems modeling expertise to the SMART Mobility consortium.

Small businesses can apply to get help from Los Alamos fuel-cell scientists to improve their fuel-cell technology and bring it into the marketplace. The Laboratory also wants to help big car companies understand how to improve their fuel cells. Each automotive company has its own program, with proprietary technology, so each company may use different pieces of what the Laboratory has to offer in different ways. By leveraging the expertise and technology present at Los Alamos and other national labs, car companies can rapidly move their fuel-cell products toward a cleaner transportation sector.

No driver necessary

Improving how cars are made and what they run on is, from an environmental standpoint, a giant step toward making the transportation system more sustainable. But what about the system itself? Truly sustainable transportation will require a switch to unmanned vehicles (popularly referred to as self-driving cars), which will be a complete paradigm shift involving changes in behavior for individuals, families, and cities. The newly formed System and Modeling for Accelerated Research in Transportation (SMART) Mobility consortium, a collaboration between the U.S. Departments of Energy and Transportation, supports national-lab research on transportation energy technologies and safety systems such as automated vehicles.

Unmanned vehicles are receiving a lot of attention these days—mostly for being hit by human-driven cars. But the reality of these vehicles is that they have the potential to streamline traffic, reduce energy consumption, improve safety, and boost quality of life. It's just hard to predict how much they will do these things before they have been deployed en masse. Los Alamos excels at uncertainty quantification and computer modeling and will, in collaboration with the NREL, bring unparalleled expertise to these efforts.

As a participant in the SMART Mobility consortium, Los Alamos will be modeling specific cities and regional settings to investigate how a shift to automated vehicles might impact human travel behavior, energy usage, city security, and greenhouse-gas emissions.

"The Lab's expertise in using computer simulations to identify important variables will help in orchestrating the shift to automated vehicles," says Joanne Wendelberger, Los Alamos scientist and liaison for the SMART Mobility consortium.

Sustainable transportation is indeed a multifaceted challenge. It will take metallurgists, chemists, geneticists, microbiologists, sociologists, computer simulators, time, money, and the will of society to make it happen. But it's inevitable. It has to be. Our current course, or rather our recently departed course, was always going to be a dead end.

—*Eleanor Hutterer*

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